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Indirect band gap and band alignment for coherently strained Si_xGe_{1-x} bulk alloys on germanium (001) substrates

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Estimates of the fundamental (indirect) band gap and band alignments of coherently strained Si_xGe_{1-x} alloys for growth on Ge(001) are given for x in the range $0 \leq x \leq 1$. The present results were obtained by combining phenomenological deformation potential theory with the self-consistent *ab initio* pseudopotential results of Van de Walle and Martin [J. Vac. Sci. Technol. B 3, 1256 (1985)]. It is found that the band gap of the coherently strained alloy has a maximum value near $x = 0.15$, where the bulk band structure changes from Ge-like to Si-like. The conduction-band discontinuity ΔE_c shows a similar behavior, having a maximum value ≈ 0.10 eV at $x = 0.15$ and changing sign for $x \gtrsim 0.32$ (i.e., type-II alignment with the Ge conduction-band edge lying higher in energy than the alloy conduction-band edge). The present results suggest that electron transfer from the Si_xGe_{1-x} alloy to the elemental Ge is to be expected if the alloy, having $x \approx 0.15$, is selectively n-type doped. Further, hole transfer from the Si_xGe_{1-x} to the elemental Ge is expected for $x \gtrsim 0.5$. It is therefore expected that high-speed complementary logic (implemented with two-dimensional conduction in elemental Ge) may be feasible for growth of (Ge,Si) strained-layer heterostructures on Ge or Ge-rich substrates.

I. INTRODUCTION

Pseudomorphic growth of Si_xGe_{1-x} strained layers on Ge(001) substrates has recently been demonstrated by Bean,[1] using molecular-beam epitaxy. Commensurate epitaxy of Si_xGe_{1-x}/Ge strained-layer heterostructures is of interest for a number of reasons. To begin, elemental Ge possesses the highest mobility for holes of the technologically important semiconductors. This fact coupled with the exceedingly high value of the low-temperature electron mobility for intrinsic Ge ($\mu_e > 10^6\,\mathrm{cm^2\,V^{-1}\,s^{-1}}$ at $T \approx 2$ K) makes Ge a potentially important material for the realization of high-speed complementary logic. Further, it should be emphasized that the production of a two-dimensional hole gas (2DHG) in an elemental component of the (Ge,Si) system can only be accomplished in the Ge, due to the nature of the valence-band offset [step up in electron energy in going from Si to Ge (Ref. 2)]. Growth on Ge (or Ge-rich substrates) is therefore of necessity if one is to investigate 2D transport in elemental Ge while avoiding the complications of vanishingly small maximum (critical) layer thicknesses, as would be obtained for growth of Ge on Si or Si-rich substrates.[3,4]

In the present paper we therefore address the issue of the effects of coherency strain on the indirect band gap and on the band alignments of Si_xGe_{1-x} alloys for growth on Ge(001) substrates, for the entire range of alloy compositions (i.e., $0 \leq x \leq 1$).

II. BAND GAPS OF COHERENTLY STRAINED (Ge,Si) HETEROSTRUCTURES ON Ge(001)

In calculating the strained band gaps, we follow the procedure developed in studies for growth of (Ge,Si) alloys on Si(001).[5] In the present case [growth on Ge(001) substrates] the alloy layers again experience a simple tetragonal distortion,[1] wherein the (Ge,Si) layers now experience a biaxial in-plane extension (tension) and a corresponding compression along the $\langle 001 \rangle$ growth direction. If one defines $\mathbf{z} \| [001]$ (i.e., along the growth direction) then the strain tensor, e_{ij}, has only diagonal elements. The assumption of a rigid Ge lattice leads to

$$e_{xx} = e_{yy} = \frac{a(\mathrm{Ge}) - b(x)}{b(x)} > 0 , \tag{1a}$$

where a(Ge) and $b(x)$ denote the unstrained lattice parameters of Ge and the Si_xGe_{1-x} alloy, respectively. The compression e_{zz} of the alloy along the growth direction may be obtained from the tetragonal distortion, i.e.,

$$e_{zz} - e_{xx} = \left[\frac{1+\nu}{1-\nu} \right] f , \tag{1b}$$

where the lattice mismatch f is defined by

$$f = \left[\frac{b(x) - a(\mathrm{Ge})}{a(\mathrm{Ge})} \right] < 0 , \tag{1c}$$

and Poisson's ratio ν varies between 0.273 for Ge to 0.280 for Si. Equations (1a)—(1c) define the compositional dependence of the alloy strain tensor. Given the components of the alloy strain tensor, the effect of strain on the indirect band gap is readily obtained using the procedure outline in Ref. 5.

In brief review, the effect of coherence strain on the fourfold-degenerate $J = \frac{3}{2}$ valence-band edge of the alloy again causes this state to split into a set of doublets (at $\mathbf{k} = 0$), which may be specified by their magnetic quantum numbers, $\pm M_J$. In the present case, the upper valence band is $(\frac{3}{2}, \pm\frac{1}{2})$ in character, with the surface of constant

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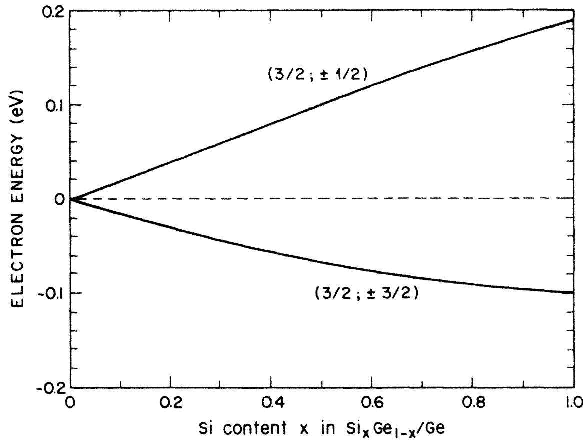

FIG. 1. Uniaxial splittings of the $J=\frac{3}{2}$ valence bands for pseudomorphic growth of Si_xGe_{1-x} alloys on Ge(001) substrates.

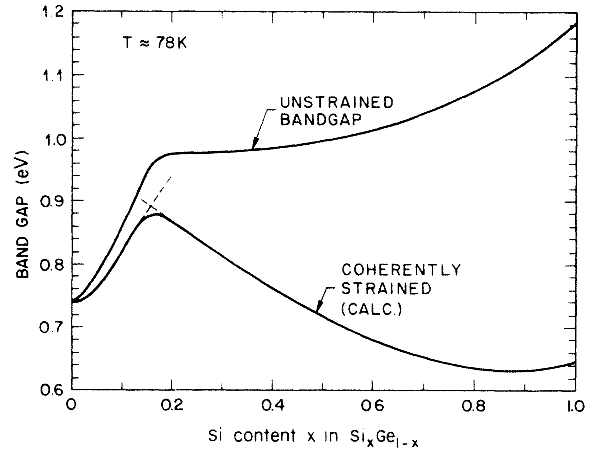

FIG. 3. Fundamental (indirect) band gap of coherently strained Si_xGe_{1-x} alloys for growth on Ge(001) substrates.

energy being an ellipsoid of revolution having its semimajor axis normal to the [001] direction in momentum space.[6] The uniaxial splittings (at $\mathbf{k}=\mathbf{0}$) of the $J=\frac{3}{2}$ valence bands are shown in Fig. 1, as a function of Si content.

In considering the uniaxial splittings of the alloy conduction-band edges, one must keep in mind the nature of the conduction-band edge as a function of alloy composition. Recall that the unstrained alloy has a Ge-like conduction-band structure (minima along $\langle 111 \rangle$ directions in momentum space) for $0 \leq x \lesssim 0.15$, whereas the conduction band of the alloy is Si-like (minima along the $\langle 001 \rangle$ directions in momentum space) for $0.15 \lesssim x \leq 1.0$;[7] for x in Si_xGe_{1-x}. It is therefore expected that the uniaxial component of the coherency strain will not cause a splitting of the alloy conduction-band edge for $0 \leq x \lesssim 0.15$, since all of the Ge-like conduction-band minima are equivalent under the effective $\langle 001 \rangle$ uniaxial stress. However, for alloys having Si-like conduction-band structure (i.e., $x \gtrsim 0.15$), the coherency strain splits the sixfold degenerate band edge into a doublet and a fourfold degenerate set of states, with the doublet being lower in energy, since $e_T < 0$ in the present case.[5] The anticipated uniaxial splittings of the alloy conduction-band edge are shown in Fig. 2.

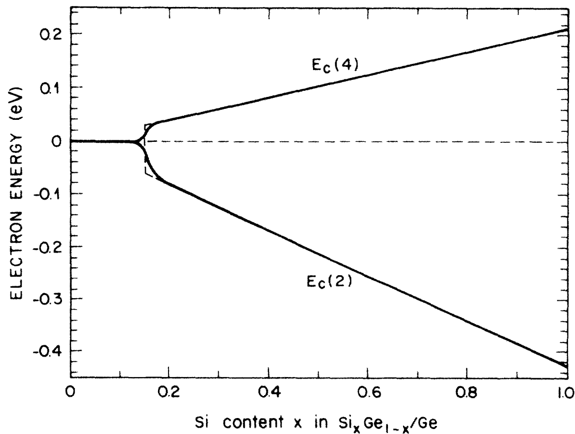

FIG. 2. Uniaxial splitting of the conduction-band minima for growth of coherently strained Si_xGe_{1-x} alloys on Ge(001) substrates.

It is further assumed that the hydrostatic deformation potential is given by the results of Paul and Warschauer,[8] i.e., that of Ge for $x \lesssim 0.15$ and that of Si for $x \gtrsim 0.15$, hence

$$\Xi_d + \frac{1}{3}\Xi_u - a = \begin{cases} -4.5\text{eV}, & 0 \leq x \lesssim 0.15 \\ +1.5\text{eV}, & 0.15 \lesssim x \leq 1 . \end{cases} \quad (2)$$

The previous assumptions, along with the unstrained band-gap data of Braunstein, Moore, and Herman[7] give the strained alloy band gap shown in the lower curve of Fig. 3. These estimates correspond to transitions from the upper most $(\frac{3}{2}, \pm\frac{1}{2})$ valence-band edge to the doubly degenerate conduction-band edge of the alloy. Note that the strained band gap is of maximum value near $x \simeq 0.15$, where the bulk band structure changes from Ge-like to Si-like. The decrease observed for $0.15 \lesssim x \lesssim 0.8$ is indicative of the fact that the reduction in band gap due to strain is larger than the increase in band gap due to increasing Si content (alloying). These two contributions are roughly equal near $x \simeq 0.9$, with the increase in band gap due to alloying outweighing the strain reductions beyond $x \simeq 0.9$.

III. BAND ALIGNMENT FOR Si_xGe_{1-x}/Ge STRAINED-LAYER HETEROSTRUCTURES ON Ge(001) SUBSTRATES

The band alignment for growth of coherently strained Si_xGe_{1-x}/Ge heterojunctions on Ge(001) is estimated by combining the strained band-gap data of Fig. 3 with the estimated valence-band offsets, ΔE_v, for the pseudomorphic interfaces. It is assumed that the effects of alloying on ΔE_v may be described by a linear interpolation.

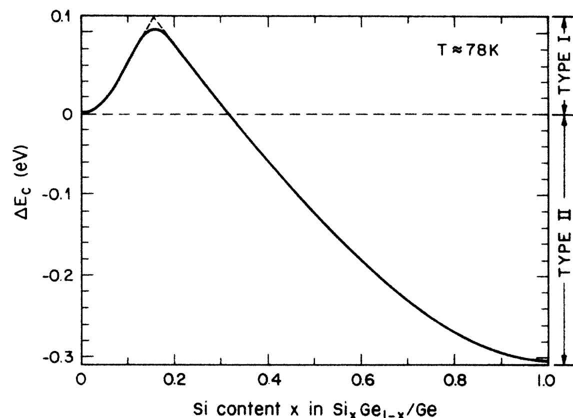

FIG. 4. Conduction-band discontinuity, ΔE_c, vs Si content (x), for pseudomorphic Si_xGe_{1-x}/Ge heterostructures on Ge(001).

This assumption, combined with the calculated ΔE_v [$\equiv E_v(\text{Ge}) - E_v(\text{Si})$] of 0.21 eV (Ref. 2) for pseudomorphic Ge/Si on Ge(001) substrates, gives (in electron energy)

$$\Delta E_v[E_v(\text{Ge}) - E_v(\text{Si}_x\text{Ge}_{1-x})] \equiv 0.21x \text{ eV} . \quad (3)$$

It is also of interest to determine the value of the conduction-band offset ΔE_c, as a function of alloy content. We define $\Delta E_c(x)$ by

$$\Delta E_c(x) \equiv E_g^{\text{strained}}(x) - E_g^{\text{cubic}}(\text{Ge}) - \Delta E_v(x) . \quad (4)$$

Note that $\Delta E_c > 0$ if the band alignment is type I, i.e., the cubic Ge band edges lie within the alloy band edges, whereas $\Delta E_c < 0$ implies a staggered (type II) band alignment in which the Ge conduction-band edge lies higher in energy than the Si_xGe_{1-x} conduction-band edge. The calculated variation of ΔE_c with Si content (x) is shown in Fig. 4. Note that ΔE_c is type I for $0 \leq x \lesssim 0.32$, and type II for $x > 0.32$.

If one is to obtain electron transfer from the alloy to the elemental Ge, then the conduction-band offset must be type I and ~ 0.10 eV. These conditions appear to be satisfied only for $x \simeq 0.15$ for growth of Si_xGe_{1-x}/Ge heterojunctions on Ge(001). Note that Eq. (3) implies that the Ge valence-band edge always lies at a higher electron energy than the Si_xGe_{1-x} valence-band edge. Therefore, if it is desirable to produce a 2D hole gas in an elemental component of the (Ge,Si) system, then this can only be accomplished in the Ge. Further, if the value of ΔE_v is to be on the order of 0.10 eV then we must have $x \simeq 0.5$, as shown in Eq. (3).

IV. SUMMARY AND CONCLUSIONS

In summary, estimates of the fundamental (indirect) band gap of Si_xGe_{1-x} alloys for pseudomorphic growth on Ge(001) substrates have been presented. These results have been combined with estimates of the valence-band offset [for the pseudomorphic Ge/Si interface and growth on Ge(001)] in order to obtain the anticipated band alignments. The effects of alloying on ΔE_v are included via a linear interpolation. It is found that the fundamental band gap of the coherently strained Si_xGe_{1-x} alloy has a maximum value near $x \approx 0.15$. A similar behavior is observed for the conduction-band offset ΔE_c, which has a maximum positive value of ~ 0.10 eV (type-I alignment) near $x = 0.15$, and becomes negative (type II staggered alignment) for $x \gtrsim 0.32$. The present results indicate that ΔE_c is of a sufficient magnitude to observe electron transfer from the Si_xGe_{1-x} to the elemental Ge for x near 0.15, when the Si_xGe_{1-x} is selectively n-type doped. Similarly, one expects to obtain a 2D hole gas in the elemental Ge for $x \approx 0.5$ and the Si_xGe_{1-x} selectively p-type doped.

Since elemental Ge has the highest hole mobility of the technologically important semiconductors and low-temperature electron mobilities in excess of $10^6 \text{cm}^2/\text{V s}$, the production of two-dimensional electron and hole gas systems in elemental Ge would be extremely exciting and would imply the feasibility of producing very high-speed complementary logic based on transport in elemental Ge.

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